Relationships between agents for modelling the intermediate stages of cement hydration

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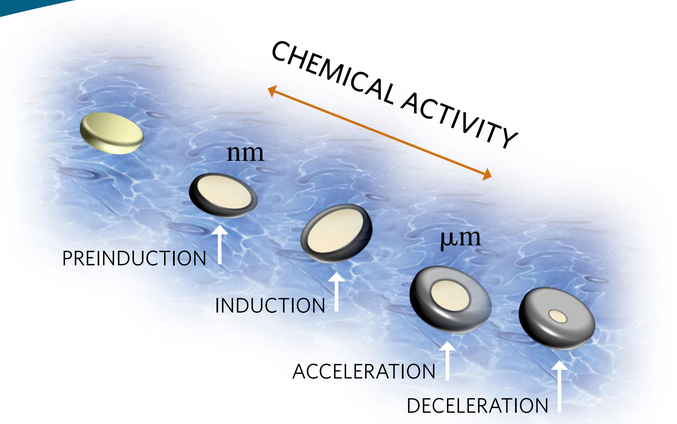
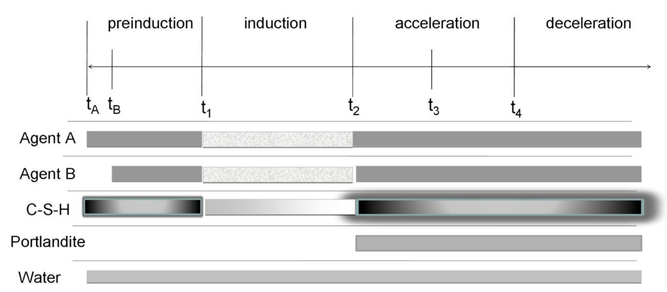
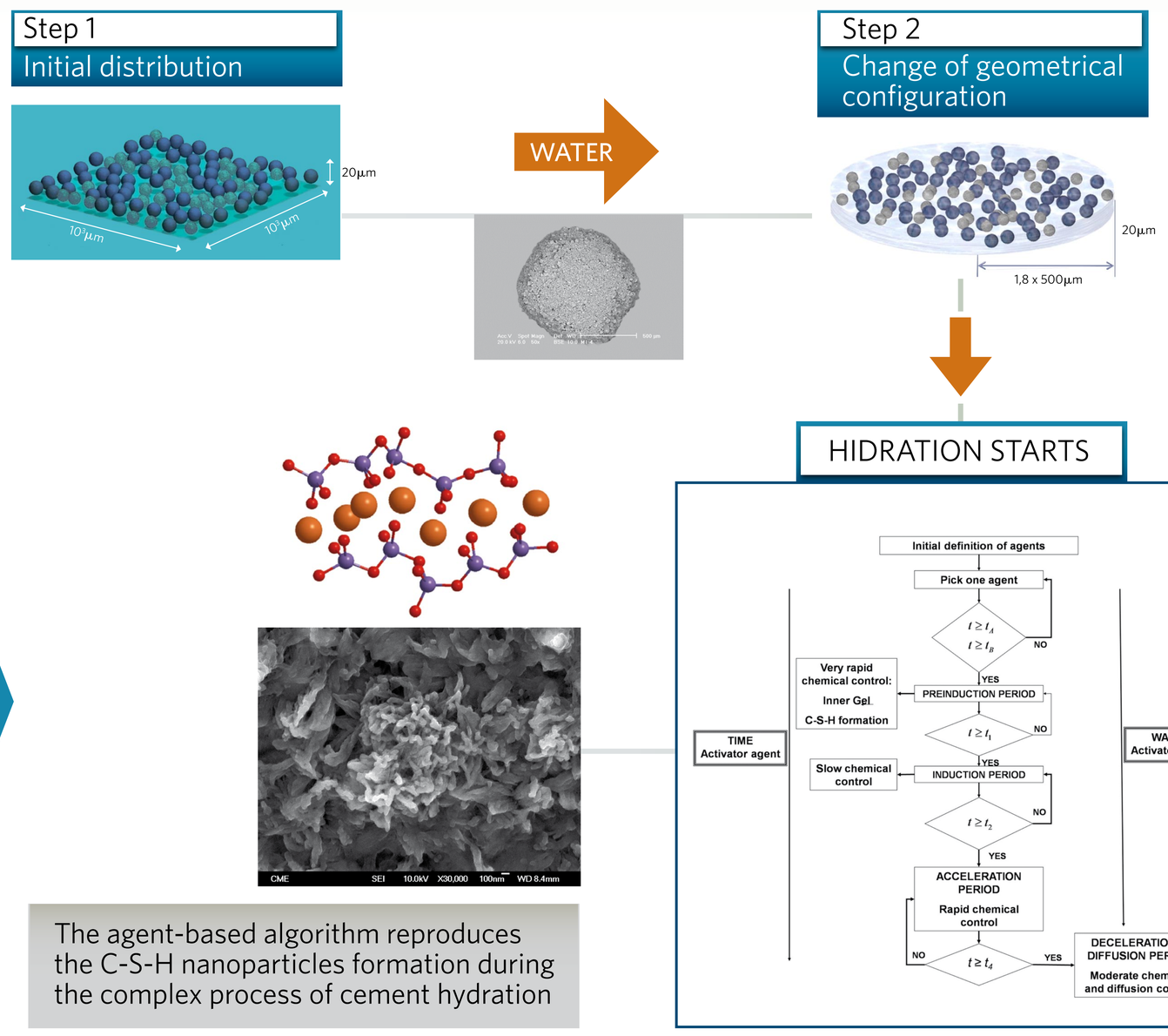


This agent-based algorithm for simulation of cement Portland hydration process at nanoscale can be helpful for better understanding and controlling the behaviour of the resulting mechanical system.

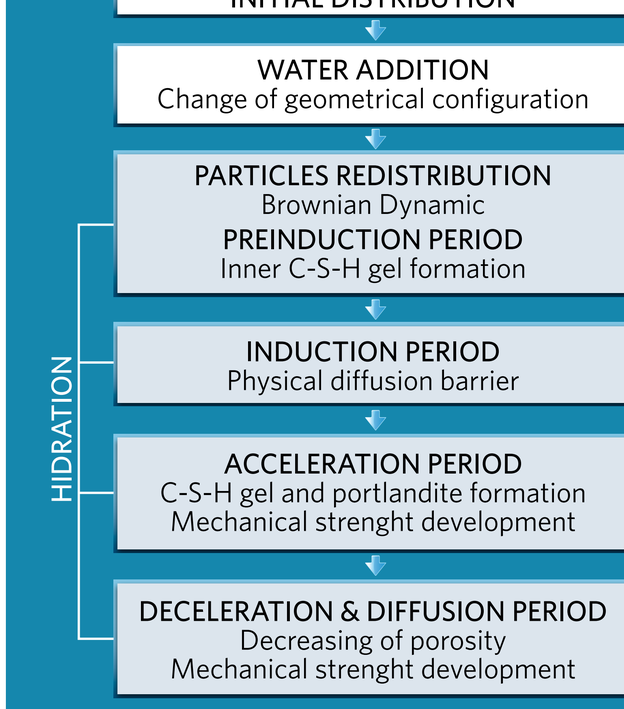


ABSTRACT

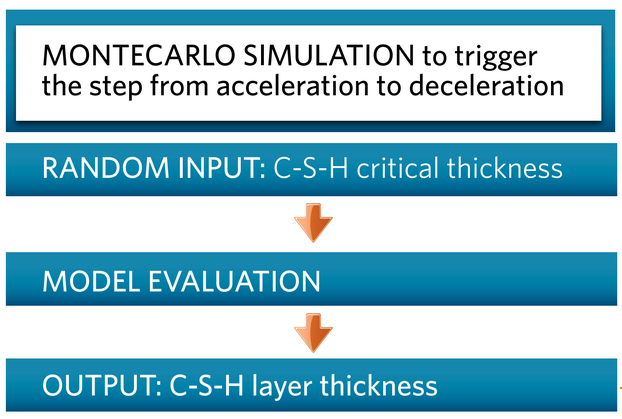
Agent-Based modelling is, in many cases, most natural for describing and simulating a system composed of "behavioral" entities. Whether one is attempting to describe the complex process of cement hydration, an agent-based approach makes the model seem closer to reality. Therefore, it is more natural to describe how the calcium silicate phases individually behave during the hydration Chemistry than to come up with the equations that govern the dynamics of the anhydrous constituents. Because the dynamic equations result from the behavior of the calcium silicate phases, the agent-based model will also enable to study aggregate properties. A model based on agents for the cement hydration, also makes it possible to analyse the formation and growing of the C-S-H gel: the main binding agent in hardened cement. Knowing the initial concentration of the anhydrous constituents makes it possible to create virtual agents which represent and behave according with their reactivity.
This work describes an algorithm which cores an agent-based approach for modelling the intermediate stages of cement hydration, focusing on the microstructure development and C-S-H gel formation. Theories relating to the mechanism of cement hydration are examined and these are discussed in terms of the agents behavioral. Monte Carlo method is applied to obtain and analyse the algorithm results.



The agent-based algorithm reproduces the C-S-H nanoparticles formation during the complex process of cement hydration



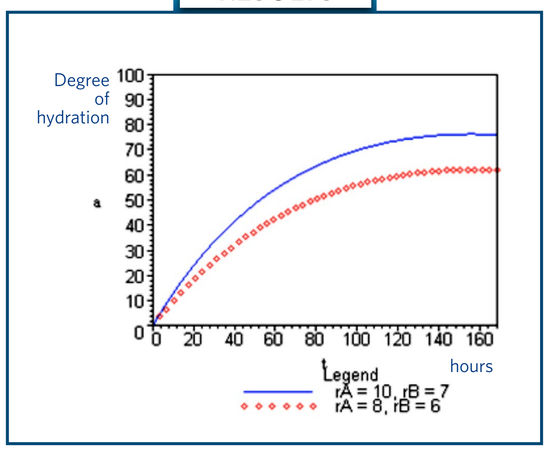
The algorithm implements stochastic, deterministic and adaptive rules that lead from a separated system to a bond system with emerging mechanical properties.



Layer thickness (in μm) of C-S-H nanoparticles precipitated on cement particles A, B respectively, during hydration process

Hydration stage	20 minutes Preinduction	28 hours Acceleration	7 days Deceleration
Particles A	0.06-0.07	4 – 5	9 – 10
Particles B	0.007-0.017	0.5 – 1.5	3 – 5

RESULTS



CONMOD 2010
22-25 June 2010
EPFL
SWITZERLAND

CONCLUSIONS

An **agent-based algorithm for simulation of cement hydration** process has been proposed, which allows to measure the degree of hydration and the thickness of C-S-H gel versus time, at early and intermediate stages. During hydration process, a critical thickness is randomly assigned to each particle within the cement past, in order to model the transition step from phase-boundary reaction to diffusion period, resulting coherent with reported experimental studies. Moreover, **Monte Carlo method** is applied to run the algorithm taking into account its random behaviour.
The **proposed model is capable of predicting the hydration kinetics of cement** under different initial conditions, resulting in good agreement with experimental results.